

3-«beta»,7-«alpha»-Dihydroxy-5-androsten-17-one

MO TMS

InChIKey:

InChI=1S/C26H47NO3Si2/c1-25-14-12-19(29-31(4,5)6)16-18(25)17-22(30-32(7,8)9)24-2

QQNSDFVOFMVHMI-VVLYNVHKSA-N

Formula:

C26H47NO3Si2

SMILES:

CON=C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

477.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	7.002		Crippen Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R386008&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/19-220-6/3-beta-7-alpha-Dihydroxy-5-androsten-17-one-MO-TMS.pdf>

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